CITRINE
INFORMATICS

White paper

3 WAYS AI SUPPORTS YOUR SUSTAINABILITY GOALS

1. Sustainable Sourcing
2. Efficient Processes
3. Green Products

3 Ways AI Supports Your Sustainability Goals

INTRODUCTION

The world's leading materials and chemicals companies now consider sustainability a business imperative. As of 2015, over 85% of chemical companies had a sustainability strategy[1], and this has likely only increased in recent years. Investors are taking action as well. In a 2019 *Harvard Business Review* article, they noted that "corporate leaders will soon be held responsible for environmental, social, and governance issues, if they aren't already." [2]

The UN has defined 17 sustainable development goals and it is undeniable that the materials and chemicals industry can have a big impact on these. New material technologies are critical to enable responsible consumption and production (goal 12), water security (6), clean energy (7), and better healthcare (3). However, the status quo for R&D often takes decades to bring new materials to market. In order to meet global sustainability needs and mitigate the impacts of global climate change, the industry must transform the way it develops materials and chemicals.

Sustainability has moved from a PR exercise to a critical factor for success in the industry. Companies have set ambitious goals around greenhouse gas emission reduction, increased energy efficiency, increasing the market share of sustainable products, and responsible raw material sourcing. In this paper, we will review how Materials Informatics can support companies striving to achieve ambitious sustainability goals.

EXAMPLES OF SUSTAINABILITY GOALS FROM INDUSTRY

	3M	DOW	ArcelorMittal	Hydro
Headline Statement	"At 3M we use our imagination to apply science to improve our planet and every life, helping to create a better future."	"Helping lead the transition to a sustainable future."	"Sustainable development is at the heart of our purpose: Inventing smarter steels for a better world."	"We believe that our future profitability depends on our ability to ensure future sustainability."
KPIS	By 2020: • Ensure GHG emissions at least 50% below our 2002 baseline • Help our customers reduce their GHGs by 250 million tons of CO2 equivalent emissions through the use of 3M products • Improve energy efficiency, indexed to net sales, by 30% • Increase renewable energy to 25% of total electricity use	• Reduce annual carbon emissions in 2030 by 5 million metric tons compared to 2020 baseline. • Collect, reuse, or recycle 1 million metric tons of plastic by 2030 • Enable 100% of plastics sold into packaging applications to be recyclable or reusable by 2035	• We have an ambitious target of a 30% reduction in CO_2 emissions in Europe by 2030 • Increase the percentage of steel made by recycling scrap • Switch to clean electricity to power furnaces	• A 30% reduction of our CO_2 emissions throughout the aluminium value chain by 2030 • Halving our non-greenhouse-gas emissions (SO_2, NOx and particulate matter only) to air. • Increase recycling of post-consumer scrap to > 250,000 mt/yr
Link to Source	3M.com	DOW.com	ARCELORMITTAL.com	HYDRO.com

[1] Making a business case for Sustainability in Chemicals, BCG report, Apr 19, 2017. https://www.bcg.com/publications/2017/making-business-case-sustainability-chemicals
[2] Shareholders are getting serious about sustainability. by Robert G. Eccles and Svetlana Klimenko, Harvard Business Review, May 2019. https://hbr.org/2019/05/the-investor-revolution

Adapt to use different feedstocks and raw materials – increase circularity and cope with shortages

METALS AND ALLOYS

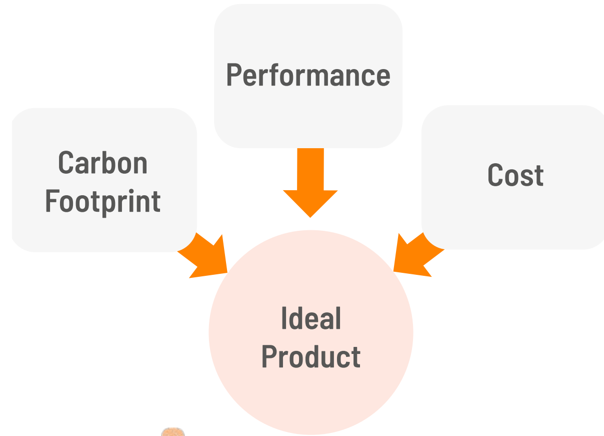
The list of critical raw materials, those elements or materials that are both crucial to the economy and have potential access issues, varies depending on your location and geopolitical connections, but most lists include some common alloying elements[3]. For companies where design, production, and maintenance in the field typically take decades, potential shortages and price volatility are a real concern. Future uncertain supply of alloying elements (Cobalt and Manganese) and even base metals (Aluminum and Titanium) is motivating the exploration of novel alloys. The market for wind turbines and electric cars will grow rapidly over the next decade, but will there be a constant supply of neodymium magnets used in the electric motors and Lithium-Ion batteries for cars?

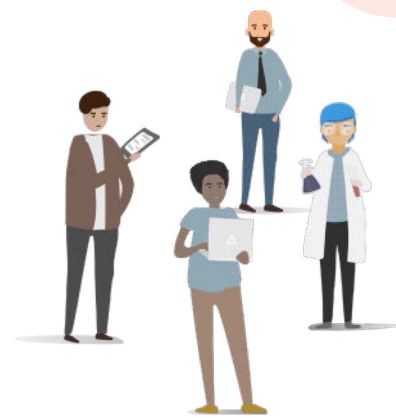
For metals and alloy producers, recycling more post-consumer scrap is energy and carbon efficient as it costs less energy to sort and remelt scrap than to start again from ores to create primary metal. However, smart processes and material science are also needed to ensure that properties are not degraded by rogue elements.

SPECIALTY CHEMICALS

Over the last 10 years lifecycle assessment methodologies have become more standardized and carbon footprint data for chemicals has become more common and comparable. This opens up the opportunity to select ingredients in a formulation based on not just cost and chemical performance, but also carbon footprint. AI enables formulation companies to create recipe banks–lists of recipes that are predicted to meet the chemical performance targets and constraints that customers require. Recipes can then be ranked by both cost and environmental impact. Companies can then have a sophisticated conversation with their customers about their needs.

Carbon footprint as a differentiator

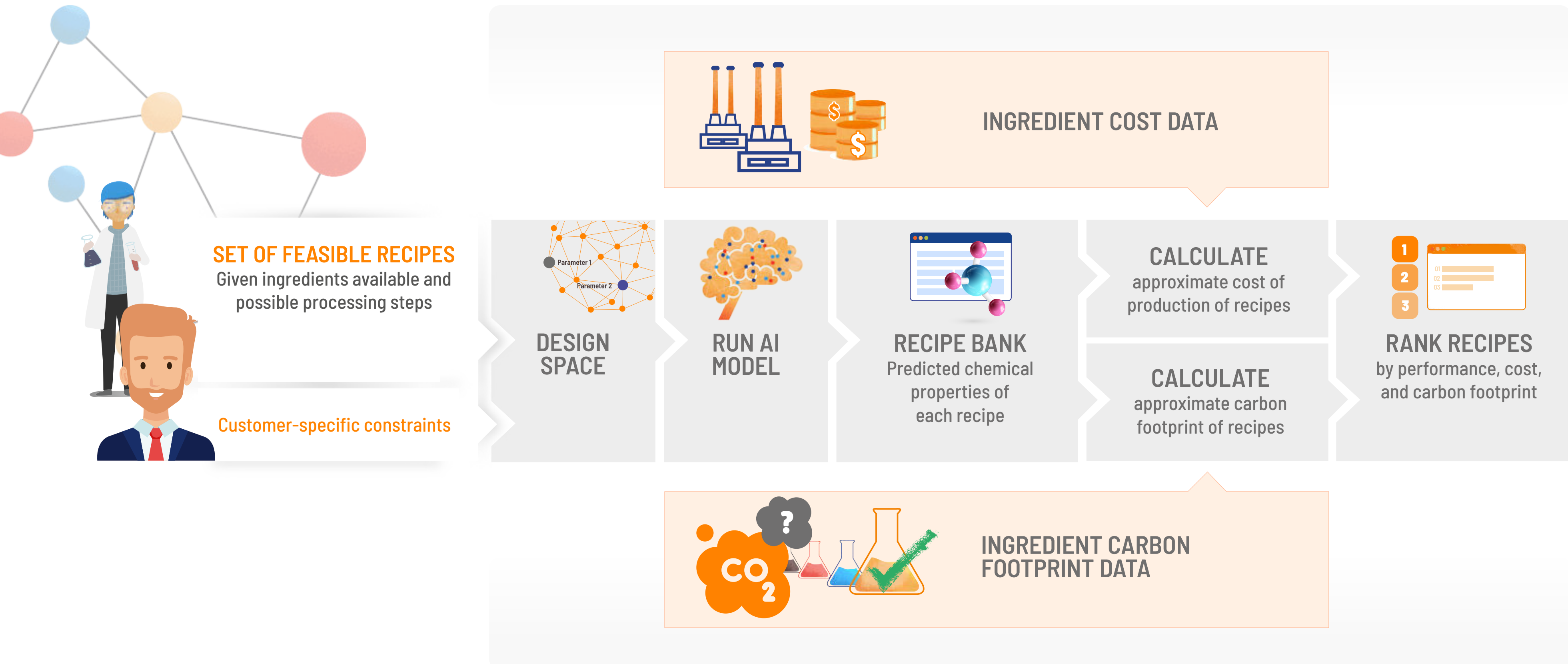




Having carbon footprint alongside performance and cost data at your fingertips, enables sophisticated negotiations with your customers.

[3] FEDERALREGISTER.gov, JIM.or.jp, RMIS.jrc.ec.europa.eu

Materials Informatics enables optimization in more dimensions



CASE STUDY – Battery materials

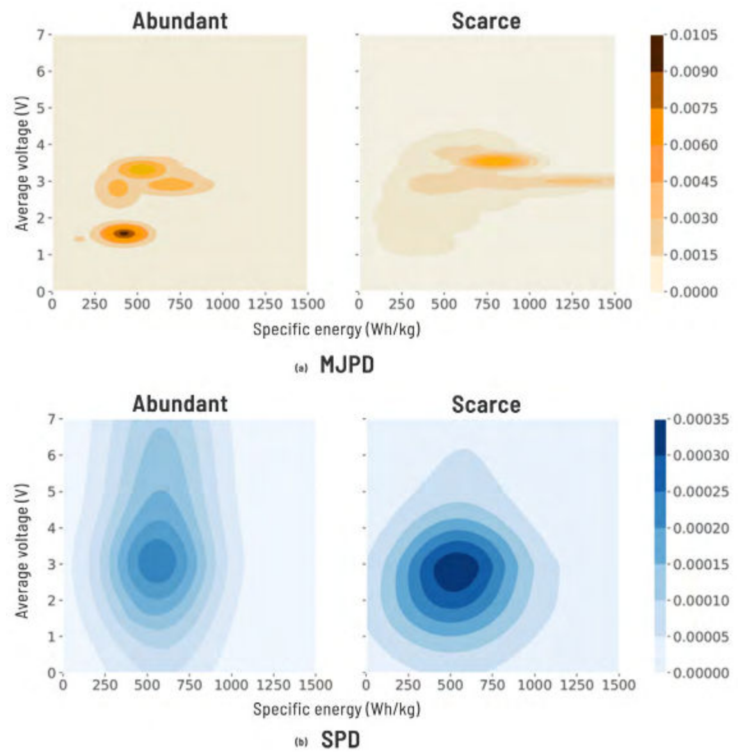
There is a societal need to improve battery materials[4] (increase specific energy while maintaining high voltage) to aid our transition to a carbon neutral economy, but battery manufacturers need secure raw material supplies[5]. Citrine ran a project to explore this trade-off.

Citrine's patented technology enables companies to understand and compare the likelihood of achieving target material properties using different design spaces (the set of material candidates whose properties are predicted by an AI model). In this project, 3 existing databases of battery materials were combined and then sorted into two groups, scarce and abundant, depending on their composition and the availability of their elements in the earth's crust. An AI model was trained and used to predict the specific energy and voltage of all the materials. Uncertainty quantification was then used to visualize the likelihood of achieving target properties in the two design spaces. The visualizations show that a higher specific energy is more likely to be achievable with cathodes that use rare elements. Research leaders can now make data-driven business decisions about whether to invest in creating test samples and performing physical testing based on market size, application, research costs, and likelihood of success. This technology can be equally applied to other sustainable sourcing considerations such as how biodegradable ingredients affect materials properties.

Trade-offs in materials properties and sustainable sourcing can be cost-effectively explored.

Details of the project can be found here: James Peerless, Emre Sevgen, Stephen Edkins, Jason Koeller (Citrine Informatics) et al. "Design space visualization for guiding investments in biodegradable and sustainably sourced materials" MRS Comms (2020)

Battery materials



Higher specific energy is more likely in materials containing rare elements

[4]Naoki Nitta, Feixiang Wu, Jung Tae Lee, Gleb Yushin, Li-ion battery materials: present and future, Materials Today, Volume 18, Issue 5, 2015, Pages 252-264, ISSN 1369-7021.
[5]H. Vikström, et al. Appl. Energy, 110 (2013), p. 252

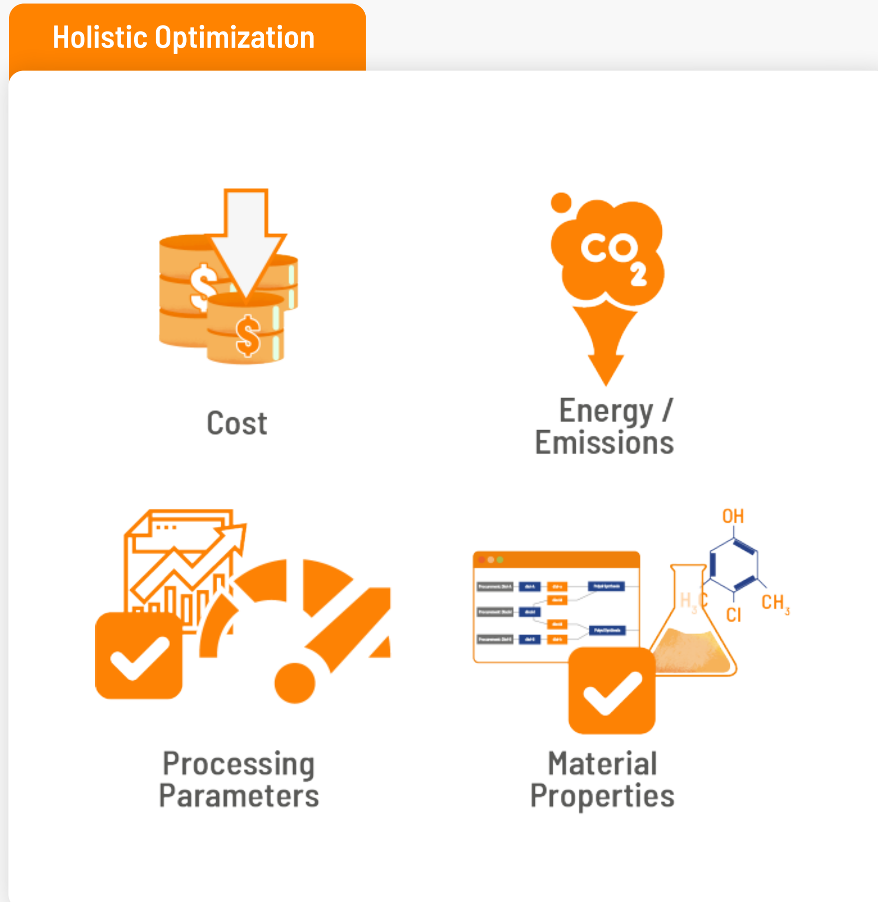
2. EFFICIENT PROCESSES

Optimize carbon footprint, energy or water use e.g. carbon capture, electrochemical processes

Many materials and chemical companies have aggressive goals to reduce their carbon footprints and their consumption of energy and water. Materials Informatics enables the analysis of thousands of different AI-generated material or chemical candidates that conform to complex constraints on processing parameters. Not only can AI reduce the number of experimental cycles, requiring less energy per project, but material candidates that meet target properties can be screened by cost and carbon footprint.

Materials and chemicals companies are switching to less carbon intensive ingredients or feedstocks and using clean electricity to power their plants. In the world of specialty chemicals, increasing both mechanical and molecular recycling of plastics are important ways to increase circularity, to satisfy both consumer buying trends and an EU European Green Deal push. Developing more effective catalysts is important for molecular recycling. Other strategies to make processing more sustainable include the development of carbon capture materials, new processes for using CO_2 as a fuel or feedstock, and developing more efficient catalysts for electrochemical reactions that can produce chemicals at room temperature.

The production of ammonia consumes 5% of global energy production and accounts for 1% of all global greenhouse gas emissions.[6]



[6] CEN.acs.org

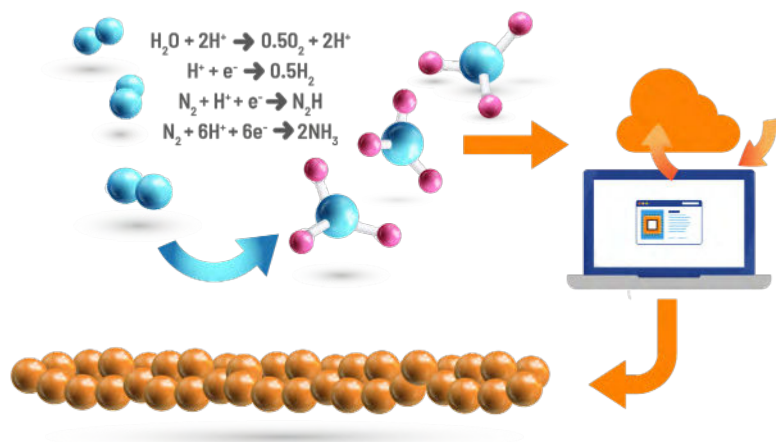
CASE STUDY – Catalysts for electrochemical processes

To accelerate the discovery of new electrochemical materials, Citrine has teamed up with research groups from Carnegie Mellon University, MIT, and Julia Computing in a US Department of Energy ARPA-E program called DIFFERENTIATE. The team's goal is to accelerate electrochemical materials development by 80% through innovating on three key fronts:

1. Software and hardware acceleration of high-fidelity simulations that predict catalyst performance
2. Surrogate models for physics-based simulations
3. A Sequential Learning–driven efficient search over a vast chemical design space to identify high-quality candidate materials in as few iterations as possible

The outcomes from this project will advance energy-efficient, sustainable methods of chemical production across a broad range of industries.

Catalysts for electrochemical processes



Accelerating development of catalysts for room temperature chemical production

Project website: CMU.edu details of the technical approach and challenges are discussed in a preprint here: arXiv:2011.04426 [cond-mat.mtrl-sci] ARXIV.org

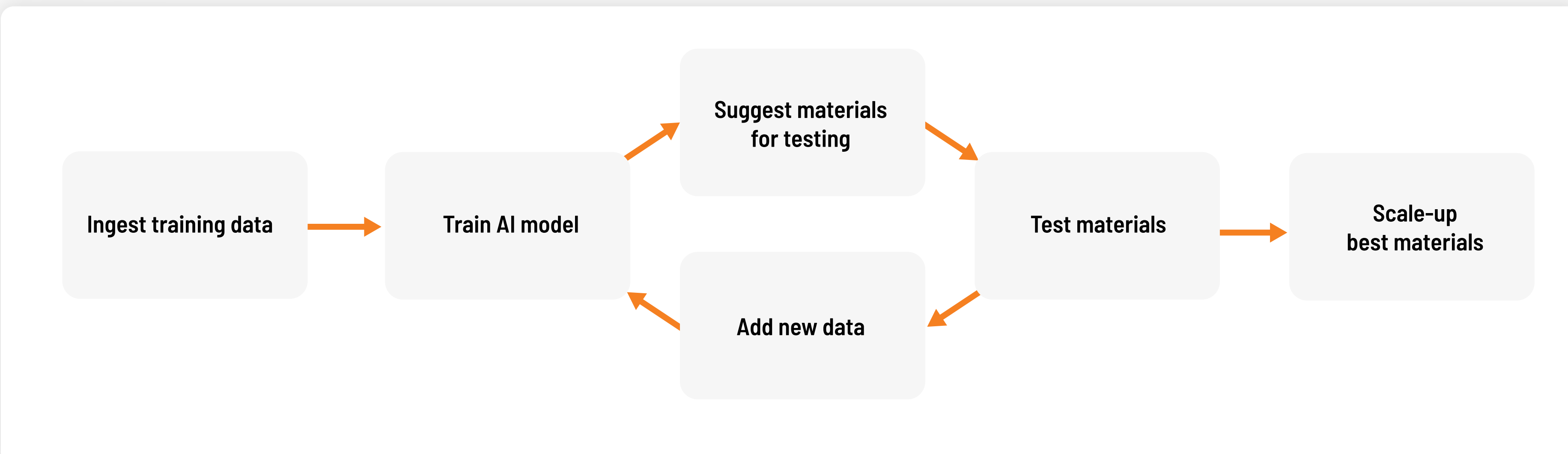
CASE STUDY – New catalyst technology – carbon capture

A leading supplier of environmental and process catalysts collaborated with Citrine on a project to identify new materials for capturing greenhouse gases, like carbon dioxide (CO_2).

Citrine trained an AI model on the customer's experimental data, which suggested better material candidates. Data from testing these candidates was combined with the original data and the model re-run and new candidates suggested. This iterative process improves the model and the quality of the material candidates suggested.

> **"The model rapidly screened thousands of new materials and became smarter in its predictions."**
>
> Leader of digitalization initiatives in heterogeneous catalysis at the customer.

Sequencial learning



3. GREEN PRODUCTS

There are growth markets for sustainable materials and chemicals that meet consumer and regulatory demand for biodegradability, low carbon footprint, or post-consumer scrap content. Materials and chemical companies can also help their customers make in-demand sustainable products by providing lightweight materials for transportation, and high-performance materials for electromobility, renewable energy and low-power lighting etc. Citrine has worked on projects across batteries, photovoltaics, and LEDs.

Materials Informatics presents a low-cost way to explore a larger design space and find novel materials

The end-of-life of plastics in particular has become a hot topic with consumers and regulators, but the same principle applies to all sorts of formulations that persist in nature. Developing formulations that are readily biodegradable means restricting the ingredients used, but will the same performance be achievable?

Materials Informatics enables a quick, low-resource way to understand trade-offs between narrowing ingredient lists and material performance

Green products

CASE STUDY – Biodegradable Consumer Products

A customer in the specialty chemicals industry wanted to reduce the long-term environmental impact of one of their products by incorporating new, biodegradable ingredients. The project optimized performance properties of a consumer product, subject to constraints on biodegradability. Measuring biodegradability takes time. In this case a transfer learning approach was leveraged to reduce the number of experimental measurements required to build accurate models. Citrine worked with the customer team to validate their hypotheses on which molecular structural features impacted their performance properties of interest and suggested experiments to guide their optimization of these properties subject to minimum biodegradability constraints.

Biodegradable products

3. GREEN PRODUCTS (cont.)

CASE STUDY – Green consumer electronics

Citrine has worked with customers across a range of electronic material, energy material, and semiconductor projects.

PHOTOVOLTAICS

The aim was to find novel materials with suitable band gaps for the application. Citrine worked with the customer team to put together a design space based on composition criteria and then develop a machine learning model to predict band gap.

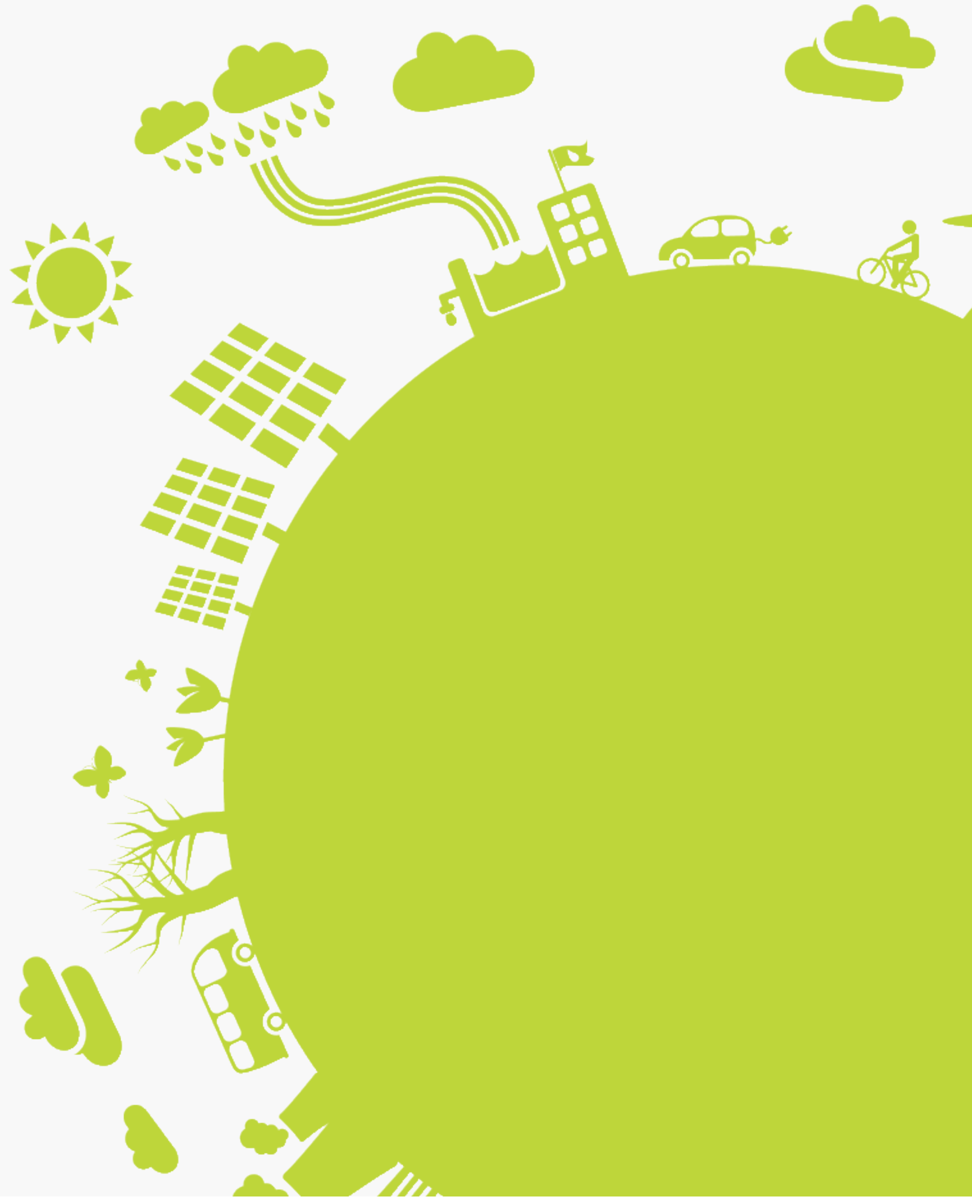
LEDs

To make low-energy LEDs a more acceptable replacement to incandescent bulbs, a customer was looking at Phosphor materials that would emit a warmer color. Citrine was able to model and predict the wavelength of emitted light based on the material composition and suggest entirely new materials to the customer team.

BATTERY MATERIALS

Citrine worked with a customer to explore the specific energy of Lithium-ion battery materials. The design space was based on the composition of the cathode with additional processing constraints. A process of Sequential Learning was used to refine the machine learning model as more data was gathered through testing candidate materials.

In each of these cases, the projects were exploratory; very little data was already available and outcomes for the projects were around finding rewarding new research directions, and more deeply understanding the correlations between input data and target properties.



SUSTAINABILITY AT CITRINE

Sustainability is important to Citrine Informatics. It is important to our founders, our investors (including Prelude Ventures, Innovation Endeavors), our employees, and increasingly our customers. For this reason, Citrine was honored to be named for a second time on the Cleantech 100 companies list in 2021. This list is compiled by an expert panel to highlight the companies that they think will have the most positive impact on climate change.

"Our mission is to accelerate the development and deployment of the next-generation of sustainable materials and chemicals. "

SUMMARY

As we all work toward a more sustainable future, we need new materials to help us solve environmental and humanitarian challenges. The materials and chemicals industry has a huge role to play, and utilizing the latest technology will enable them to succeed. AI and Materials Informatics, can increase the agility of research and development, speeding up the time it takes to develop new materials, while optimizing processing and materials properties at the same time. It can help us to find novel new materials and understand trade-offs between restricted ingredient sets and material performance. It is a vital tool for companies looking to reduce emissions and resource intensity, increase circularity, and adapt to a changing world while developing higher-margin, sustainable products.

Contact us to find out more about our technology and how we can help your business become more sustainable.

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